

Binary Classification Based on Potential Functions

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Binary classification is a type of machine learning that focuses on the task of classifying the members of a given set of objects into two groups on the basis of whether they have some property or not. Some computational methods of binary classification include decision trees, Bayesian networks, support vector machines (SVM), and neural networks. Applications of binary classification can range from simple geometric tests to significant problems of practical interest in medicine.

Suppose that $\{\mathbf{y}_i\}_{i=1}^m$ is a set of data of one type, that we will call *positive* and $\{\mathbf{z}_i\}_{i=1}^n$ is a data set of another type that we call *negative*. Together we call these sets the *training data*. Suppose that both sets of data are vectors in \mathbb{R}^N . We will assume that \mathbb{R}^N decomposes into two sets Y and Z such that each $\mathbf{y}_i \in Y$, $\mathbf{z}_i \in Z$ and any point in Y should be classified as positive and any point in Z should be classified as negative. Suppose that $\mathbf{x} \in \mathbb{R}^N$ and we wish to predict whether \mathbf{x} belongs to Y or Z using only information from the finite sets of data $\{\mathbf{y}_i\}$ and $\{\mathbf{z}_i\}$. Given distance functions $d_1(\cdot, \cdot)$ and $d_2(\cdot, \cdot)$ and positive constants $\{a_i\}_{i=1}^m$, $\{b_i\}_{i=1}^n$, α and β we define a potential function:

$$I(\mathbf{x}) = \sum_{i=1}^m \frac{a_i}{d_1(\mathbf{x}, \mathbf{y}_i)^\alpha} - \sum_{i=1}^n \frac{b_i}{d_2(\mathbf{x}, \mathbf{z}_i)^\beta}.$$

If $I(\mathbf{x}) > 0$ then we say that I classifies \mathbf{x} as belonging to Y and if $I(\mathbf{x})$ is negative then \mathbf{x} is classified as part of Z . The constants, $\{a_i\}_{i=1}^m$, $\{b_i\}_{i=1}^n$, α and β and even the distance functions $d_1(\cdot, \cdot)$ and $d_2(\cdot, \cdot)$ can be determined from the training data.

The potential method of binary classification, as presented here, is observed to be computationally trivial while retaining a high level of accuracy that can compete with and even surpass that of the popular SVM methods. This method can be shown to be an extension of the nearest neighbor methods. The training data can be weighted based on distances to a decision surface, and the method can be further extended to account for anticipated feature correlations.

The potential method was tested on a 4 by 4 checkerboard and two clinical micro-array data sets for which the performance of the SVM methods is known. Leave one out cross validation (LOOCV) was used to train and test the classifier on the two micro-array data sets. For these data sets, LOOCV has been shown to be a valid methodology [1]. The results achieved demonstrate that, despite its relative simplicity, the potential method can be just as effective as the SVM methods in binary classification. There are possible optimizations to this method including improvements of the implementation of weights and multi-variable optimizations. Although all optimizations are to some extent dependent on the data sets studied, it was observed that the optimization is stable over a large range. This algorithm is also easily parallelized, which is certainly attractive with current trends in technology.

[1] A. Statnikov, C.F. Aliferis, I. Tsamardinos, D. Hardin, S. Levy, A Comprehensive Evaluation of Multicategory Classification Methods for Microarray Gene Expression Cancer Diagnosis, *Bioinformatics* **21**(5), 631-43, 2005.